

Intrinsic spin orbit torque in a single domain nanomagnet

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We present theoretical studies of the intrinsic spin orbit torque (SOT) in a single domain ferromagnetic layer with Rashba spin-orbit coupling (SOC) using the non-equilibrium Green's function formalism for a model Hamiltonian. We find that, to the first order in SOC, the intrinsic SOT has only the field-like torque symmetry and can be interpreted as the longitudinal spin current induced by the charge current and Rashba field. We analyze the results in terms of the material related parameters of the electronic structure, such as band filling, band width, exchange splitting, as well as the Rashba SOC strength. On the basis of these numerical and analytical results, we discuss the magnitude and sign of SOT. Our results show that the different sign of SOT in identical ferromagnetic layers with different supporting layers, e.g. Co/Pt and Co/Ta, could be attributed to electrostatic doping of the ferromagnetic layer by the support.

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I. INTRODUCTION

Magnetization switching in nanoscale devices induced by electric currents has been a subject of intensive studies in recent years.¹ One of the most scrutinized approaches is the transfer of spin angular momentum between non-collinear ferromagnetic layers, an effect known as spin transfer torque (STT).^{2,3} In this case, the charge current is spin polarized by a magnetic layer with a pinned magnetization and the spin angular momentum is deposited in a free layer causing precession and reversal of the magnetization. Recently, an alternative way to produce spin torque and manipulate the magnetization direction in a ferromagnetic layer was demonstrated, as it does not require the presence of a second polarizing ferromagnet. Instead, it is produced by spin-orbit coupling (SOC).⁴⁻⁶ This spin-orbit torque (SOT) was observed in 3d ferromagnets grown on 5d materials with strong SOC, such as Pt^{4,5,7,8} or Ta.^{6,9,10} In this setup, the charge current flows in the plane parallel to the interface and SOT has been shown to produce domain wall motion^{11,12} and magnetization precession.^{13,14} Moreover, recent studies reported on a giant SOT arising at the interface between a topological insulator and ferromagnet¹⁵ or another magnetically-doped topological insulator.¹⁶

The presence of SOT in single nanomagnets has been predicted theoretically based on analytical models.^{17,18} Two principal mechanisms of SOT have been proposed. The first mechanism is based on the Rashba effect at the interface between a ferromagnetic layer and supporting non-magnetic metal with strong SOC. The charge current passing through the ferromagnet produces intrinsic torques due to Rashba SOC.^{4,5,17-21} The second mechanism is based on the bulk spin Hall effect (SHE) in the support. In this case, the charge current pass-

ing through the support produces spin accumulation at the interface which exerts SOT on the magnetization in a ferromagnet.^{6,7,22,23} The particular experimental setup determines which of the two mechanisms dominates. The observation of a strong dependence of the SOT magnitude on the support thickness and its sign reversal at small thicknesses¹⁰ suggest that for a thick supporting layer the current flows predominantly through the support and the SHE-SOT dominates. On the other hand, when the support is very thin the current flows through the ferromagnetic layer and the Rashba-SOT dominates.

Many theoretical works employ a picture of conduction electrons interacting with localized magnetic moments in the presence of Rashba SOC¹⁷⁻²¹ or SHE.^{22,23} The conduction electrons are assumed to be free and their interaction with localized moments is treated on the level of the *s-d* exchange model.^{24,25} In the context of transport calculations, the majority of works deal with the quasi-classical Boltzmann approach.^{17,18,20,22,23} All these approaches assume linear regime, in which SOT is proportional to the charge current and the torque is expressed in terms of phenomenological parameters, such as the spin Hall angle and spin polarization of the carriers. There is also a couple of reports on first-principles calculations of SOT, where the torque is related to the Berry phase curvature of the occupied states.^{26,27} Nevertheless, the band structure dependence and the finite bias behavior of SOT remain largely unexplored.

In this paper, we focus on the study of intrinsic mechanisms of SOT based on the ballistic transport theory within the Keldysh non-equilibrium Greens function (NEGF) formalism and tight binding (TB) Hamiltonian model for a ferromagnetic layer with Rashba spin-orbit coupling. To gain insights into physical picture, we derive an analytic expression for SOT in the first order of SOC

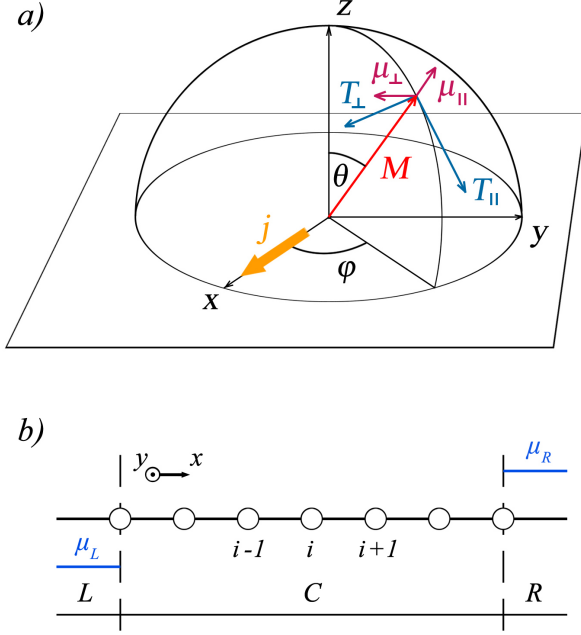


FIG. 1. a) Schematic view of the 2D ferromagnetic layer in the xy plane. The charge current \mathbf{j} direction is along the x -axis. The magnetization \mathbf{M} is defined by the spherical angles θ and ϕ . The purple arrows indicate the current-induced electron spin density. The blue arrows denote \mathbf{T}_\perp and \mathbf{T}_\parallel contributions to the total SOT. b) Schematic view of the two-probe setup consisting of the scattering region C and two electrodes L and R .

and use it to analyze the SOT dependence on the band structure parameters and applied voltage. We show that the first order in SOC terms leads to the FLT component.

II. METHODOLOGY

We consider a two dimensional ferromagnetic layer in the so-called current-in-plane (CIP) geometry schematically shown in Fig. 1a. The direction of the charge current \mathbf{j} is chosen to be along the x axis and the unit vector \mathbf{S} along the magnetization \mathbf{M} is given in the conventional spherical coordinate system, $\mathbf{S} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta)$. The induced SOT can be separated into two components which have symmetries of the damping-like, \mathbf{T}_\parallel , and field-like, \mathbf{T}_\perp , torques given by the directions of the magnetization \mathbf{S} and applied charge current \mathbf{j} as $\mathbf{T}_\parallel = T_\parallel \mathbf{S} \times [(\mathbf{e}_z \times \mathbf{j}) \times \mathbf{S}]$ and $\mathbf{T}_\perp = T_\perp (\mathbf{e}_z \times \mathbf{j}) \times \mathbf{S}$, where \mathbf{e}_z is the unit vector along the z axis.

A. Hamiltonian matrix elements

The Hamiltonian of the system in the absence of SOC is

$$\hat{\mathcal{H}}_0 = \sum_{nm,\sigma} t_{nm} \hat{c}_n^{+\sigma} \hat{c}_m^\sigma - j_{ex} \sum_{n,\sigma\sigma'} \hat{c}_n^{+\sigma'} (\boldsymbol{\sigma} \cdot \mathbf{S})^{\sigma'\sigma} \hat{c}_n^\sigma, \quad (1)$$

where the first term corresponds to the conduction electrons with diagonal elements representing the onsite energies, $\varepsilon_0 = t_{nn}$, and off-diagonal elements representing the electron hopping parameters, $t_{n,m \neq n}$. We consider the hopping parameter to be non-zero between nearest neighbors only, $t = t_{n,n+1} = t_{n+1,n}$. The second term is the so-called s - d model, where j_{ex} stands for the exchange coupling and $\boldsymbol{\sigma}$ is the vector of the Pauli matrices.^{24,25} The Rashba SOC Hamiltonian is written in the tight-binding basis as²⁸

$$\hat{\mathcal{H}}_{SO} = -\lambda \sum_{n,\sigma\sigma'} \left[\hat{c}_{n+\mathbf{e}_y}^{+\sigma'} (i\sigma_x^{\sigma'\sigma}) \hat{c}_n - \hat{c}_{n+\mathbf{e}_x}^{+\sigma'} (i\sigma_y^{\sigma'\sigma}) \hat{c}_n + \text{H.C.} \right], \quad (2)$$

where λ is the Rashba SOC strength, \mathbf{e}_x and \mathbf{e}_y are the unit vectors in the x and y axes respectively.

The equations above can be Fourier transformed and written in the momentum space as

$$\hat{\mathcal{H}}_0(\mathbf{k}) = \begin{pmatrix} \varepsilon_0 - j_{ex} \cos \theta + t p(\mathbf{k}) & -j_{ex} \sin \theta e^{-i\phi} \\ -j_{ex} \sin \theta e^{i\phi} & \varepsilon_0 + j_{ex} \cos \theta + t p(\mathbf{k}) \end{pmatrix} \quad (3)$$

and

$$\hat{\mathcal{H}}_{SO}(\mathbf{k}) = -\lambda \begin{pmatrix} 0 & r(\mathbf{k}) \\ r^*(\mathbf{k}) & 0 \end{pmatrix}, \quad (4)$$

where $p(\mathbf{k}) = 2(\cos k_x + \cos k_y)$ and $r(\mathbf{k}) = 2(i \sin k_x + \sin k_y)$. Finally, the total Hamiltonian of the system is $\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{\mathcal{H}}_{SO}$.

B. Non-equilibrium charge and spin transport for current-in-the-plane geometry

In order to calculate transport properties we separate the system into three regions along the x axis, a scattering region (C) connected to the left (L) and right (R) semi-infinite leads all made of the same material (Fig 1b). The choice of the scattering region dimensions is arbitrary, as long as it is large enough so that all properties of interest are independent of its size. A finite voltage drop $eV = \mu_L - \mu_R$ is introduced between the leads by maintaining them in local thermodynamic equilibrium with chemical potentials $\mu_{L(R)}$. Thus, the occupation of the leads is governed by the Fermi-Dirac distribution function $f_{L(R)} = 1/(1 + e^{(E - \mu_{L(R)})/k_B T})$. The system is assumed to be periodic in the y direction perpendicular to the current.

In this setup, the charge and spin current densities between any two neighboring planes i and $i+1$ in the x direction are given in the NEGF formalism as²⁹

$$I = \frac{e}{\hbar} \int \frac{dE dk_y}{4\pi^2} \text{Tr}_\sigma [\hat{\mathcal{H}}_{i,i+1} \hat{G}_{i+1,i}^<(E, k_y) - \hat{\mathcal{H}}_{i+1,i} \hat{G}_{i,i+1}^<(E, k_y)] \quad (5)$$

and

$$\mathbf{I}^S = \int \frac{dE dk_y}{8\pi^2} \text{Tr}_\sigma [(\hat{\mathcal{H}}_{i,i+1} \hat{G}_{i+1,i}^<(E, k_y) - \hat{\mathcal{H}}_{i+1,i} \hat{G}_{i,i+1}^<(E, k_y)) \boldsymbol{\sigma}], \quad (6)$$

where all quantities are 2×2 matrices in the spin space, $\mathcal{H}_{i,i+1}$ is the Hamiltonian matrix element between the planes i and $i+1$, and $G_{i,i+1}^<$ is the NEGF. The integration is performed over the energy and y component of the wave vector \mathbf{k} .

Similarly the spin density of conduction electrons arising from the s - d exchange coupling is given by³⁰

$$\boldsymbol{\mu} = -i\mu_B \int \frac{dE dk_y}{8\pi^2} \text{Tr}_\sigma [\hat{G}_{i,i}^<(E, k_y) \boldsymbol{\sigma}], \quad (7)$$

where μ_B is the Bohr magneton. All quantities are independent of the plane index i . Having calculated the magnetic moment, the spin torque can be readily found as

$$\mathbf{T} = -\frac{j_{ex}}{\mu_B} \mathbf{S} \times \boldsymbol{\mu}. \quad (8)$$

C. Non-equilibrium Green's function matrix elements

The NEGF for a standard two-probe geometry can be written in the form^{31,32}

$$\hat{G}^< = i\hat{G}(f_L \hat{\Gamma}_L + f_R \hat{\Gamma}_R) \hat{G}^+, \quad (9)$$

where \hat{G} is the retarded Green's function (GF), $\hat{\Gamma}_{L(R)} = i(\hat{\Sigma}_{L(R)} - \hat{\Sigma}_{L(R)}^+)$ is the escape rate to the electrodes, $\hat{\Sigma}_{L(R)}^+ = \hat{\mathcal{H}}_{L(R)C}^+ \hat{g}_{LL(RR)} \hat{\mathcal{H}}_{L(R)C}$ is the self-energy due to the attachment of the electrodes, and $\hat{g}_{LL(RR)}$ is the surface GF of the electrode.

Due to the periodicity along the y axes, the retarded GF matrix elements can be written in the mixed (real and reciprocal space) representation as the Fourier transform of GF, $\hat{G}(\mathbf{k})$, in momentum space

$$\hat{G}_{n,m}(k_y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x e^{ik_x(n-m)} \hat{G}_{nm}(\mathbf{k}), \quad (10)$$

where $\hat{G}(\mathbf{k}) = [(E + i\eta)\hat{I} - \hat{\mathcal{H}}(\mathbf{k})]^{-1}$, η is a positive infinitesimal, n and m are layer indexes along the x axis.

The surface GF of the electrodes can be found from the bulk GF, because connecting two semi-infinite systems restores an infinite periodic system.³³ For the self-energies we obtain $\hat{\Sigma}_L = \hat{G}_{i+j,i+1}^{-1} \hat{G}_{i+j,i} \hat{\mathcal{H}}_{i,i+1}$ and $\hat{\Sigma}_R = \hat{G}_{i,i+j}^{-1} \hat{G}_{i,i+j+1} \hat{\mathcal{H}}_{i+1,i}$, where $i \in (-\infty, \infty)$ and $j \in [1, \infty)$. Since the bulk GF is periodic, its matrix elements depend only on the difference of their coordinates, $\hat{G}_{n,m} = \hat{G}_{n-m}$. Thus, substituting into Eq. (9) we obtain

$$\hat{G}_{i,j}^< = -f_L \hat{G}_{i+1,i} \hat{\mathcal{H}}_{i,i+1} \hat{G}_{i,i}^+ + f_L \hat{G}_{i,i} \hat{\mathcal{H}}_{i+1,i} \hat{G}_{i+1,i}^+ - f_R \hat{G}_{i,i+1} \hat{\mathcal{H}}_{i+1,i} \hat{G}_{i,i}^+ + f_R \hat{G}_{i,i} \hat{\mathcal{H}}_{i+1,i} \hat{G}_{i+1,i}^+. \quad (11)$$

Finally, taking into account an explicit form of the Hamiltonian matrix elements $\hat{\mathcal{H}}_{i,i+1} = \hat{I}t - i\lambda\hat{\sigma}_y$ and using $\hat{\mathcal{H}}_{i+1,i}^+ = \hat{\mathcal{H}}_{i,i+1}$, the diagonal NEGF matrix element can be written as

$$\begin{aligned} \hat{G}_{i,i}^< &= f_L t (\hat{G}_{i,i} \hat{G}_{i+1,i}^+ - \hat{G}_{i+1,i} \hat{G}_{i,i}^+) \\ &+ f_R t (\hat{G}_{i,i} \hat{G}_{i+1,i}^+ - \hat{G}_{i+1,i} \hat{G}_{i,i}^+) \\ &+ i f_L \lambda (\hat{G}_{i,i} \hat{\sigma}_y \hat{G}_{i+1,i}^+ + \hat{G}_{i+1,i} \hat{\sigma}_y \hat{G}_{i,i}^+) \\ &- i f_R \lambda (\hat{G}_{i,i+1} \hat{\sigma}_y \hat{G}_{i,i}^+ + \hat{G}_{i,i} \hat{\sigma}_y \hat{G}_{i+1,i}^+). \end{aligned} \quad (12)$$

Using this expression, the non-equilibrium spin density $\boldsymbol{\mu}$ [Eq. (7)] and SOT [Eq. (8)] can be calculated in general. Nevertheless, in order to obtain deeper insight in the behavior of SOT, we can expand the NEGF matrix elements in orders of the SOC strength λ . The somewhat lengthy algebra is given in Appendix A. The main result is that the spin density can be decomposed into two components, as follows

$$\boldsymbol{\mu} = \boldsymbol{\mu}_\parallel + \boldsymbol{\mu}_\perp = \mathbf{S}(\mu_0 + 2S_y\mu_1) + (0, -2\mu_1, 0), \quad (13)$$

where μ_0 and μ_1 are the zeroth and first orders in the expansion in λ . From Eq. (8) it is clear that only the second term produces SOT, $\mathbf{T} = T_\perp (S_z, 0, -S_x)$, which has the field-like symmetry, where

$$T_\perp = -\frac{2j_{ex}\mu'}{\mu_B} = \frac{\hbar\lambda}{et} (I^\uparrow - I^\downarrow) = \frac{2\lambda}{t} I^{S_z}, \quad (14)$$

Thus we find that, for the intrinsic SOT arising from Rashba SOC, the damping-like term appears in the second order of the SOC strength compared to its field-like counterpart, i.e. $T_\perp \gg T_\parallel$. This result is in agreement with previous studies which show that the interface SOC results in predominantly field-like torques.^{26,27} This SOT can be interpreted as the longitudinal spin current induced by the charge current and SOC.

III. RESULTS AND DISCUSSION

We start with selecting parameters of the tight-binding model. Many experimental studies use Co or CoFe as the ferromagnetic layer and Pt or Ta as the support.^{6,9,17} Thus, the ferromagnetic material is either Fe or Co,

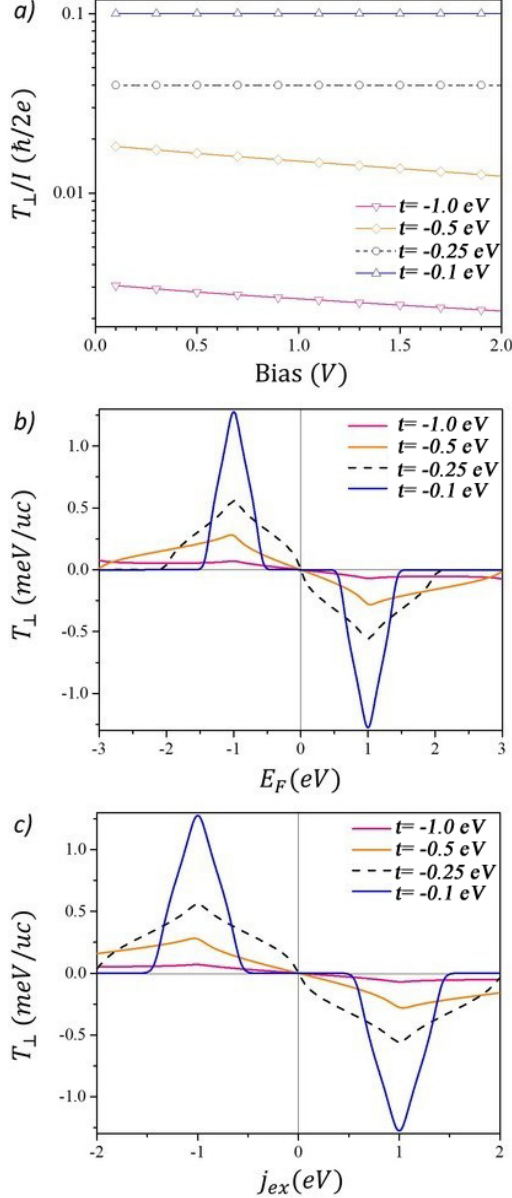


FIG. 2. a) Bias dependence of the SOT efficiency for different values of the electron hopping parameter ($j_{ex} = 1.0$ eV, $\lambda = 0.01$ eV and $E_F = 1.0$ eV); b) SOT dependence on the Fermi level ($j_{ex} = 1.0$ eV, $\lambda = 0.01$ eV and $V = 0.1$ V); c) SOT dependence on the exchange interaction parameter for different values of the electron hopping parameter ($E_F = 1.0$ eV, $\lambda = 0.01$ eV and $V = 0.1$ V).

which have very similar band structures but differ by one electron in occupation. Within the s - d exchange model, centers of the majority and minority bands are at $\varepsilon^{\uparrow} = \varepsilon_0 - j_{ex}$ and $\varepsilon^{\downarrow} = \varepsilon_0 + j_{ex}$, respectively. The exchange splitting between two bands is $2j_{ex}$ and the band width is $8t$. Thus, for $|j_{ex}/t| < 4$ the material has a gap between the majority and minority bands. For a typical

ferromagnet, such as Co or Fe, the exchange splitting is of the order of a couple of eV and the band width is of the order of several eV. Therefore, this band structure can be described by choosing $j_{ex} = 1.0$ eV and $t = -1.0$ eV, respectively, which is representative for a metallic ferromagnet with the exchange splitting of 2.0 eV. Note that for $j_{ex} = 1.0$ eV, the case of $t < -0.25$ eV is an insulator. Without any loss of generality, we set the onsite energy $\varepsilon_0 = 0.0$ eV, while the band occupation is controlled by shifting the Fermi level E_F . We also choose $\lambda = 0.01$ eV for the SOC strength.

Using this parametrization, we calculate SOT from Eq. (14) and plot in Fig. 2a the SOT efficiency as a ratio of SOT to the charge current, T_{\perp}/I . The Fermi level is chosen at $E_F = -1.0$ eV, which corresponds to the half-filled majority band and completely empty minority band. For comparison between the metallic ($t = -1.0$ eV) and insulating ($t = -0.1$ eV) cases, we also plot the SOT efficiency for several different band widths. The main observation is that the SOT efficiency decreases exponentially with the band width. Another observation is that SOT is fairly independent of the bias. Because of the choice of E_F , only the majority band contributes to the transport, $I^{\uparrow} \neq 0$ and $I^{\downarrow} = 0$, as a result SOT is proportional to the current and the SOT efficiency is constant. At higher bias, the minority band also contributes to the charge current, and the overall efficiency and SOT decrease when the current increases.

In order to gather deeper insight into the origin of SOT we investigate its dependency on the main parameters of the model, i.e. band filling and exchange splitting. In Fig. 2b the dependence on the band occupation is shown for different band widths. The applied bias is set to $V = 0.1$ V. As it is seen, SOT is an antisymmetric function with respect to E_F . The magnitude of T_{\perp} peaks around the middle of the majority and minority bands at $\varepsilon_0 - E_F = \mp 1.0$ eV, respectively. The contributions to SOT come only from the energy regions with available carriers, therefore, for an insulating system SOT has two narrow peaks around the band centers. The maximum SOT values correspond to the 1/4 and 3/4 filled bands. It is worth to notice that in the area of 1/2 filling the sign of T_{\perp} can change for small charge doping shifting of E_F to the left or right. This fact can explain the difference in the sign of SOT for the cases of Co/Pt and Co/Ta.⁹ Chemically, Co (or CoFe) is between Ta and Pt in electronegativity. Thus, the interface with Pt is going to dope the ferromagnetic slab with holes, while the interface with Ta with electrons. Since the ferromagnetic layer is very thin this doping will change the Fermi level position of the whole system. It could be sufficient to make the transport majority- or minority-dominated, that, in turn, changes the sign of SOT.

In Fig. 2c the dependence of T_{\perp} on the exchange splitting is shown. SOT is an odd function of j_{ex} that is easily explained by switching the order of the majority and minority band positions when the exchange interaction changes between ferromagnetic and antiferromag-

netic. Thus, the sign of SOT, in principle, also depends on the exchange coupling of the ferromagnet itself and could be different in different materials. It is also seen that SOT is a non-monotonous function of j_{ex} , that is not obvious, as intuitively it is expected that larger exchange couplings lead to larger SOT. However, SOT reaches its maximum (minimum) value at the same j_{ex} for all curves. This value of j_{ex} corresponds to the case when one of the spin-channels gives the highest contribution.

IV. CONCLUSIONS

We have presented analytical and numerical results for SOT in single domain ferromagnets with Rashba SOC. We have showed that in the first order in SOC this torque corresponds to the FLT symmetry and is proportional to the longitudinal component of the spin-current. The analytical expression of SOT is given in terms of the material related parameters of the electronic structure that enables physically more transparent analysis. Our results indicate that the SOT efficiency decreases with the band width and it has maxima at 1/4 and 3/4 band fillings. At the same time, for band fillings close to 1/2 the sign of SOT can be changed by a small electrostatic doping. Thus, experimental observations of opposite signs of SOT in Co/Pt and Co/Ta layers could be explained in terms of the hole and electron doping of the Co layer from the supporting Pt or Ta layers, respectively. We expect that our results would be a useful tool to select specific material combinations with optimal properties.

Finally, we would like to point out that recent theoretical predictions based on the non-equilibrium Green's function formalism and showed that low charge currents flowing solely in the interface of a ferromagnetic layer and topological insulator can induce antidamping-like SOTs.³⁶ Nevertheless, the antidamping-like SOT that is of particular importance in magnetization switching was recently observed in the ferromagnetic semiconductor (Ga,Mn)As, and its intrinsic origin was attributed to the Berry curvature, in analogy to the origin of the intrinsic SHE.³⁷ This disagreement with the Berry phase theory has to be the subject of future studies.

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Appendix A: Perturbation expansion in SOC parameter

If we consider the zeroth order with respect to the SOC parameter, Eq. (12) can be simplified as

$$\hat{G}_{i,i}^{<(0)} = f_L t (\hat{g}_{i,i} \hat{g}_{i+1,i}^+ - \hat{g}_{i+1,i} \hat{g}_{i,i}^+) + f_R t (\hat{g}_{i,i} \hat{g}_{i+1,i}^+ - \hat{g}_{i+1,i} \hat{g}_{i,i}^+), \quad (\text{A1})$$

where \hat{g} is the GF in the absence of SOC. Its explicit angular dependence is given by

$$\begin{aligned} g^{\uparrow\uparrow} &= \frac{1}{2}(g^{\uparrow}(1 + \cos \theta) + g^{\downarrow}(1 - \cos \theta)), \\ g^{\downarrow\downarrow} &= \frac{1}{2}(g^{\uparrow}(1 - \cos \theta) + g^{\downarrow}(1 + \cos \theta)), \\ g^{\uparrow\downarrow} &= \frac{1}{2}(g^{\uparrow} - g^{\downarrow}) \sin \theta e^{-i\phi}, \\ g^{\downarrow\uparrow} &= \frac{1}{2}(g^{\uparrow} - g^{\downarrow}) \sin \theta e^{i\phi}, \end{aligned} \quad (\text{A2})$$

and $g^{\uparrow(\downarrow)}$ is the GF corresponding to the case when the magnetization is perpendicular to the plane (or in the local coordinate frame aligned with the magnetization \mathbf{S}). For $t < 0$ its analytical expression is

$$\begin{aligned} g_{i,j}^{\sigma}(k_y) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \frac{e^{ik_x(x_i - x_j)}}{E^{\sigma} - 2t \cos k_x + i\eta} \\ &= -i \frac{\left(\frac{E^{\sigma}}{2t} + i\sqrt{1 - \left(\frac{E^{\sigma}}{2t} \right)^2} \right)^{|x_i - x_j|}}{\sqrt{4t^2 - E^{\sigma 2}}}, \end{aligned} \quad (\text{A3})$$

where $E^{\uparrow(\downarrow)} = E - \varepsilon_o \pm j_{ex} - 2t \cos k_y$. The matrix elements of $\hat{G}_{i,i}^{<(0)}$ are then given by

$$\begin{aligned} G_{i,i}^{<\uparrow\uparrow(0)} &= -it(f_L + f_R) \text{Im}[(g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} + g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \\ &\quad + (g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} - g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \cos \theta], \\ G_{i,i}^{<\downarrow\downarrow(0)} &= -it(f_L + f_R) \text{Im}[(g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} + g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \\ &\quad - (g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} - g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \cos \theta], \\ G_{i,i}^{<\uparrow\downarrow(0)} &= -it(f_L + f_R) \text{Im}[(g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} \\ &\quad - g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \sin \theta e^{-i\phi}], \\ G_{i,i}^{<\downarrow\uparrow(0)} &= -it(f_L + f_R) \text{Im}[(g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} \\ &\quad - g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \sin \theta e^{i\phi}]. \end{aligned} \quad (\text{A4})$$

The magnetic moment arising due to the s - d exchange coupling in the absence of SOC can be written as

$$\begin{aligned} \mu_0 &= -\mu_B t \int \frac{dE dk_y}{4\pi^2} (f_L + f_R) \\ &\quad \times \text{Im}(g_{i+1,i}^{\uparrow} g_{i,i}^{\uparrow*} - g_{i+1,i}^{\downarrow} g_{i,i}^{\downarrow*}) \mathbf{S} \\ &= -\mu_B \int \frac{dE dk_y}{4\pi^2} (f_L + f_R) \text{Im}(g_{i,i}^{\uparrow} - g_{i,i}^{\downarrow}) \mathbf{S}. \end{aligned} \quad (\text{A5})$$

This magnetic moment is collinear to the magnetization and, therefore, it does not create any torques. In equilibrium $f_L = f_R = f(E_F)$, and we obtain

$$\begin{aligned}\boldsymbol{\mu}_0 &= -\mu_B t \int \frac{dE dk_y}{2\pi^2} f(E_F) \text{Im}(g_{i,i}^\uparrow - g_{i,i}^\downarrow) \mathbf{S} \\ &= \mu_B (\langle n_i^\uparrow \rangle - \langle n_i^\downarrow \rangle) \mathbf{S},\end{aligned}\quad (\text{A6})$$

where $\langle n_i^\sigma \rangle = \int dE \rho_i^\sigma(E) f(E_F)$ is the average number of s -electrons of spin σ at atom i , and ρ is the density of states (DOS).

Let us define the charge and z -component of the spin currents given by Eqs. (5) and (6) in the absence of SOC with respect to the local coordinate frame aligned with the magnetization \mathbf{S}

$$\begin{aligned}I &= \frac{et}{\hbar} \int \frac{dE dk_y}{4\pi^2} [G_{i+1,i}^{<\uparrow\uparrow(0)} - G_{i,i+1}^{<\uparrow\uparrow(0)} \\ &\quad + G_{i+1,i}^{<\downarrow\downarrow(0)} - G_{i,i+1}^{<\downarrow\downarrow(0)}], \\ I^{S_z} &= \int \frac{dE dk_y}{8\pi^2} [G_{i+1,i}^{<\uparrow\uparrow(0)} - G_{i,i+1}^{<\uparrow\uparrow(0)} \\ &\quad - G_{i+1,i}^{<\downarrow\downarrow(0)} + G_{i,i+1}^{<\downarrow\downarrow(0)}].\end{aligned}\quad (\text{A7})$$

Using Eqs. (A4) and (A2) we obtain

$$\begin{aligned}I &= \frac{et}{\hbar} \int \frac{dE dk_y}{4\pi^2} [\theta(4t^2 - E^{\uparrow 2}) + \theta(4t^2 - E^{\downarrow 2})], \\ I^{S_z} &= \int \frac{dE dk_y}{8\pi^2} [\theta(4t^2 - E^{\uparrow 2}) - \theta(4t^2 - E^{\downarrow 2})],\end{aligned}\quad (\text{A8})$$

where $\theta(t)$ is the Heaviside step function. Integration with respect to k_y yields $I = I^\uparrow + I^\downarrow$ and $I^{S_z} = \frac{\hbar}{2e} (I^\uparrow - I^\downarrow)$, where

$$I^\sigma = \frac{e}{\hbar} \int_{-\infty}^{\infty} \frac{dE}{2\pi} (f_L - f_R) D^\sigma(E) \quad (\text{A9})$$

and

$$\begin{aligned}D^\sigma(E) &= \theta(16t^2 - (E - \varepsilon^\sigma)^2) [\theta(4t^2 - (E - \varepsilon^\sigma + 2t)^2) \\ &\quad + \frac{1}{\pi} \arccos\left(\frac{E - \varepsilon^\sigma - 2t}{2t}\right) \theta\left(\frac{E - \varepsilon^\sigma}{t}\right) \\ &\quad - \frac{1}{\pi} \arccos\left(\frac{E - \varepsilon^\sigma + 2t}{2t}\right) \theta\left(-\frac{E - \varepsilon^\sigma}{t}\right)].\end{aligned}$$

Here I^σ is the contribution of the charge current from the channel with spin σ , D^σ is the corresponding transmission function, and $\varepsilon^\sigma = \varepsilon_o \pm j_{ex}$. Note that in the limit of low temperatures the integral for D^σ can be taken analytically.

Next, we collect the terms of Eq. (12) with the first power of λ

$$\begin{aligned}\hat{G}_{i,i}^{<(1)} &= f_L t \left(\hat{g}_{i,i} \hat{G}_{i+1,i}^{(1)+} + \hat{G}_{i,i}^{(1)} \hat{g}_{i+1,i}^+ - \hat{g}_{i+1,i} \hat{G}_{i,i}^{(1)+} - \hat{G}_{i+1,i}^{(1)} \hat{g}_{i,i}^+ \right) \\ &\quad + f_R t \left(\hat{g}_{i,i} \hat{G}_{i,i+1}^{(1)+} + \hat{G}_{i,i}^{(1)} \hat{g}_{i,i+1}^+ - \hat{g}_{i,i+1} \hat{G}_{i,i}^{(1)+} - \hat{G}_{i,i+1}^{(1)} \hat{g}_{i,i}^+ \right) \\ &\quad + i f_L \lambda (\hat{g}_{i,i} \sigma_y \hat{g}_{i+1,i}^+ + \hat{g}_{i+1,i} \sigma_y \hat{g}_{i,i}^+) \\ &\quad - i f_R \lambda (\hat{g}_{i,i} \sigma_y \hat{g}_{i,i+1}^+ + \hat{g}_{i,i+1} \sigma_y \hat{g}_{i,i}^+),\end{aligned}\quad (\text{A10})$$

where $\hat{G}^{<(1)}$ stands for the GF's correction to the first order in SOC

$$\hat{G}_{nm}^{<(1)}(k_y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \hat{g}(\mathbf{k}) \hat{\mathcal{H}}_{SO}(\mathbf{k}) \hat{g}(\mathbf{k}) e^{ik_x(n-m)}. \quad (\text{A11})$$

Having substituted $\hat{G}^{<(1)}$ in Eq. (A11), we obtain the final expression for the on-site matrix elements of $\hat{G}_{i,i}^{<(1)}$

$$\begin{aligned}G_{i,i}^{<\uparrow\uparrow(1)} &= i\lambda(f_R - f_L) \left[\frac{1}{t} \text{Re}(g_{i,i}^\uparrow + g_{i,i}^\downarrow) \sin \theta \cos \phi \right. \\ &\quad \left. + \frac{1}{2} \text{Re}[(\Lambda_1 + \Lambda_2 - \frac{1}{t}(g_{i,i}^\uparrow + g_{i,i}^\downarrow)) \sin 2\theta \sin \phi] \right], \\ G_{i,i}^{<\uparrow\downarrow(1)} &= \lambda(f_R - f_L) [(\sin^2 \theta \sin^2 \phi - 1) \text{Re}[\Lambda_1 + \Lambda_2] \\ &\quad + \frac{i}{2} \text{Re}[\Lambda_1 + \Lambda_2 - \frac{1}{t}(g_{i,i}^\uparrow - g_{i,i}^\downarrow)] \sin^2 \theta \sin 2\phi \\ &\quad - \frac{1}{t} \text{Re}(g_{i,i}^\uparrow + g_{i,i}^\downarrow) \sin^2 \theta \sin^2 \phi], \\ G_{i,i}^{<\downarrow\uparrow(1)} &= \lambda(f_R - f_L) [(1 - \sin^2 \theta \sin^2 \phi) \text{Re}[\Lambda_1 + \Lambda_2] \\ &\quad + \frac{i}{2} \text{Re}[\Lambda_1 + \Lambda_2 - \frac{1}{t}(g_{i,i}^\uparrow - g_{i,i}^\downarrow)] \sin^2 \theta \sin 2\phi \\ &\quad + \frac{1}{t} \text{Re}(g_{i,i}^\uparrow + g_{i,i}^\downarrow) \sin^2 \theta \sin^2 \phi], \\ G_{i,i}^{<\downarrow\downarrow(1)} &= i\lambda(f_R - f_L) \left[\frac{1}{t} \text{Re}(g_{i,i}^\uparrow + g_{i,i}^\downarrow) \sin \theta \cos \phi \right. \\ &\quad \left. - \frac{1}{2} \text{Re}[(\Lambda_1 + \Lambda_2 - \frac{1}{t}(g_{i,i}^\uparrow + g_{i,i}^\downarrow)) \sin 2\theta \sin \phi] \right],\end{aligned}\quad (\text{A12})$$

where

$$\begin{aligned}\Lambda_1 &= g_{i,i}^{\uparrow*} (g_{i+1,i}^\downarrow - 2tK), \\ \Lambda_2 &= g_{i,i}^{\downarrow*} (g_{i+1,i}^\uparrow - 2tK), \\ K &= \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x g^\uparrow(\mathbf{k}) g^\downarrow(\mathbf{k}) \sin^2 k_x.\end{aligned}$$

Since all matrix elements of $\hat{G}^{<(1)}$ are proportional to the difference between the Fermi-Dirac functions of the left and right leads, they vanish in equilibrium. Following the definition of Eq. (7), we can write the current-induced contribution $\boldsymbol{\mu}_1$ to the magnetic moment to the first order in λ

$$\begin{aligned}\mu_{1x} &= \mu_1 \sin^2 \theta \sin 2\phi, \\ \mu_{1y} &= 2\mu_1 (\sin^2 \theta \sin^2 \phi - 1), \\ \mu_{1z} &= \mu_1 \sin 2\theta \sin \phi,\end{aligned}\quad (\text{A13})$$

where the coefficient μ_1 depends on the band structure and applied bias

$$\mu_1 = -\frac{\mu_B \lambda}{4\pi^2} \int dE dk_y (f_L - f_R) \text{Re}[\Lambda_1 + \Lambda_2]. \quad (\text{A14})$$

It can be further simplified

$$\text{Re}[\Lambda_1 + \Lambda_2] = \frac{1}{2t j_{ex}} (\theta(4t^2 - E^{\uparrow 2}) - \theta(4t^2 - E^{\downarrow 2})),$$

that yields

$$\begin{aligned}\mu_1 &= -\frac{\mu_B \lambda}{8\pi^2 t j_{ex}} \int dE (f_L - f_R) (D^\uparrow(E) - D^\downarrow(E)) \\ &= -\frac{\mu_B \lambda \hbar}{2et j_{ex}} (I^\uparrow - I^\downarrow).\end{aligned}\quad (\text{A15})$$

Finally, the total magnetic moment $\boldsymbol{\mu}$ in the first order of SOC can be written

$$\boldsymbol{\mu} = \boldsymbol{\mu}_\parallel + \boldsymbol{\mu}_\perp = \mathbf{S}(\mu_0 + 2S_y \mu_1) + (0, -2\mu_1, 0), \quad (\text{A16})$$

where only the second term leads to SOT, which is of the field-like symmetry,

$$\mathbf{T} = T_\perp (S_z, 0, -S_x) \quad (\text{A17})$$

and

$$T_\perp = -\frac{2j_{ex}\mu_1}{\mu_B} = \frac{\hbar\lambda}{et} (I^\uparrow - I^\downarrow). \quad (\text{A18})$$

Appendix B: Equation of motion for the spin density

Generally, the result given above can be derived directly from the equation of motion for the spin density. The spin current operator in the second quantization is

$$\hat{\mathbf{j}}_{i \rightarrow j}^S = -\frac{i}{4} \sum_{\sigma\sigma'} \left(\hat{c}_j^{+\sigma'} \{ \boldsymbol{\sigma}, \tilde{t}_{ji} \}^{\sigma'\sigma} \hat{c}_i^\sigma - \text{H.C.} \right), \quad (\text{B1})$$

where $\{ \boldsymbol{\sigma}, \tilde{t}_{ji} \}$ is the symmetrized product of the Pauli matrices and tight-binding Hamiltonian of a general form

$$\hat{\mathcal{H}} = \sum_{ij, \sigma\sigma'} \tilde{t}_{ij}^{\sigma\sigma'} \hat{c}_i^{+\sigma} \hat{c}_j^{\sigma'}.$$

In the absence of SOC, the Hamiltonian $\hat{\mathcal{H}}_0$ [Eq. (1)] produces the well-known 'kinetic' contribution to the spin current

$$\begin{aligned}\hat{j}_{i \rightarrow j}^{S_x} &= -\frac{it}{2} (\hat{c}_j^{+\uparrow} \hat{c}_i^\downarrow + \hat{c}_j^{+\downarrow} \hat{c}_i^\uparrow - \hat{c}_i^{+\uparrow} \hat{c}_j^\downarrow - \hat{c}_i^{+\downarrow} \hat{c}_j^\uparrow), \\ \hat{j}_{i \rightarrow j}^{S_y} &= -\frac{t}{2} (\hat{c}_j^{+\uparrow} \hat{c}_i^\downarrow - \hat{c}_j^{+\downarrow} \hat{c}_i^\uparrow - \hat{c}_i^{+\uparrow} \hat{c}_j^\downarrow + \hat{c}_i^{+\downarrow} \hat{c}_j^\uparrow), \\ \hat{j}_{i \rightarrow j}^{S_z} &= -\frac{it}{2} (\hat{c}_j^{+\uparrow} \hat{c}_i^\uparrow - \hat{c}_j^{+\downarrow} \hat{c}_i^\downarrow - \hat{c}_i^{+\uparrow} \hat{c}_j^\uparrow + \hat{c}_i^{+\downarrow} \hat{c}_j^\downarrow),\end{aligned}\quad (\text{B2})$$

while the SOC part of the Hamiltonian $\hat{\mathcal{H}}_{SO}$ [Eq. (2)] gives rise to the SOC-induced spin currents with the only non-zero components

$$\begin{aligned}\hat{j}_{SO, i \rightarrow i+e_x}^{S_x} &= \lambda \hat{\rho}_{i, i+e_x}, \\ \hat{j}_{SO, i \rightarrow i+e_y}^{S_y} &= -\lambda \hat{\rho}_{i, i+e_y},\end{aligned}\quad (\text{B3})$$

where $\hat{\rho}_{ij} = \frac{1}{2} \sum_\sigma (\hat{c}_j^{+\sigma} \hat{c}_i^\sigma + \text{H.C.})$.

Starting from equation of motion for the spin density operator in a Heisenberg picture

$$\frac{d\hat{\mathbf{s}}_i}{dt} = -\frac{i}{\hbar} [\hat{\mathbf{s}}_i, \hat{\mathcal{H}}] \quad (\text{B4})$$

with $\hat{\mathbf{s}}_i = \frac{\hbar}{2} \sum_{\sigma\sigma'} \hat{c}_i^{+\sigma'} \boldsymbol{\sigma}^{\sigma'\sigma} \hat{c}_i^\sigma$, we obtain³⁴

$$\frac{d\hat{\mathbf{s}}_i}{dt} + \text{div } \hat{\mathbf{j}}_i^S - j_{ex} \hat{\mathbf{s}}_i \times \mathbf{S} = \hat{\mathbf{j}}_i^\omega, \quad (\text{B5})$$

where $\hat{\mathbf{j}}_i^\omega$ is given by

$$\begin{aligned}\hat{j}_i^{\omega_x} &= \frac{\lambda}{t} (\hat{j}_{i \rightarrow i+e_x}^{S_z} + \hat{j}_{i-e_x \rightarrow i}^{S_z}), \\ \hat{j}_i^{\omega_y} &= \frac{\lambda}{t} (\hat{j}_{i \rightarrow i+e_y}^{S_z} + \hat{j}_{i-e_y \rightarrow i}^{S_z}), \\ \hat{j}_i^{\omega_z} &= \frac{\lambda}{t} (\hat{j}_{i \rightarrow i+e_x}^{S_x} + \hat{j}_{i-e_x \rightarrow i}^{S_x} + \hat{j}_{i \rightarrow i+e_y}^{S_y} + \hat{j}_{i-e_y \rightarrow i}^{S_y})\end{aligned}\quad (\text{B6})$$

and reflects the fact that spin is not a conserved quantity in the presence of SOC which acts as a magnetic field forcing spin to precession.³⁵

Taking statistical averages of the spin density in a steady state gives

$$\langle \text{div } \hat{\mathbf{j}}_i^S \rangle - j_{ex} \langle \hat{\mathbf{s}}_i \times \mathbf{S} \rangle = \langle \hat{\mathbf{j}}_i^\omega \rangle.$$

For the sake of simplicity, we consider the magnetization lying in the xz plane, $\mathbf{S} = (\sin \theta, 0, \cos \theta)$, and the spin polarized current flowing along the x axis. In a ballistic regime, the divergence of the spin current is close to zero on a macroscopic scale, when the system is large enough so that all inhomogeneities are negligible. In the first order of SOC, we can also neglect all the induced currents flowing along the transverse y direction. However, one should take into account that the non-collinearity between $\hat{\mathbf{s}}_i$ and \mathbf{S} in the first order of SOC is driven by the transverse component of the spin current, that is $\hat{j}_{i \rightarrow i+e_y}^{S_z}$, and according to Eq. (B6) only \hat{s}_y produces SOT with the non-zero x and z components

$$\begin{aligned}-j_{ex} \langle \hat{\mathbf{s}}_y \rangle S_z &= \frac{2\lambda}{t} \langle \hat{j}_{i \rightarrow i+e_x}^{S_z} \rangle, \\ j_{ex} \langle \hat{\mathbf{s}}_y \rangle S_x &= \frac{2\lambda}{t} \langle \hat{j}_{i \rightarrow i+e_x}^{S_x} \rangle,\end{aligned}\quad (\text{B7})$$

respectively. All the averages in this equation can be expressed through NEGF $\hat{G}_{i,j}^< = i \langle \hat{c}_j^\dagger \hat{c}_i \rangle$. Taking into account Eqs. (7) and (8), and substituting $\langle \hat{j}_{i \rightarrow i+e_x}^{S_z} \rangle = I^{S_z} \cos \theta$ and $\langle \hat{j}_{i \rightarrow i+e_x}^{S_x} \rangle = I^{S_z} \sin \theta$ (after a transformation to the global coordinate frame), we finally obtain

$$\begin{aligned}\mathbf{T}_\perp &= \frac{2\lambda}{t} I^{S_z} (S_z, 0, -S_x) \\ &= \frac{\hbar\lambda}{et} (I^\uparrow - I^\downarrow) (S_z, 0, -S_x),\end{aligned}\quad (\text{B8})$$

that is the same result obtained in Appendix A.

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